

Probabilites in the general boundary formulation

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Abstract. We give an introductory account of the general boundary formulation of quantum theory. We refine its probability interpretation and emphasize a conceptual and historical perspective. We give motivations from quantum gravity and illustrate them with a scenario for describing gravitons in quantum gravity.

1. A geometric-algebraic approach to quantum theory

Since we want to contrast the general boundary formulation with the standard formulation of quantum theory, we should state precisely what we mean by the latter. Firstly, there is a *time* variable $t \in \mathbb{R}$ which is classical and provided from the outset. Secondly, there is a Hilbert space \mathcal{H} of *states*. In the Schrödinger picture, which we will use, a state is thought to encode the physical condition of the system under consideration at a given time. Thirdly, a state evolves in time according to a dynamical law. The time evolution from time t_1 to time t_2 is encoded in an operator $U(t_1, t_2) : \mathcal{H} \rightarrow \mathcal{H}$. For consistency we must have $U(t_2, t_3)U(t_1, t_2) = U(t_1, t_3)$ for any $t_1 < t_2 < t_3$. We will refer to this as the *composition rule*. Note that we may describe $U(t_1, t_2)$ through its matrix elements, i.e., *transition amplitudes*. We write the transition amplitude from an initial state ψ at time t_1 to a final state η at time t_2 as usual as $\langle \eta | U(t_1, t_2) | \psi \rangle$. Fourthly, the modulus square of a transition amplitude encodes a probability in a measurement process: $|\langle \eta | U(t_1, t_2) | \psi \rangle|^2$ encodes the probability of measuring the state η at time t_2 given that the state ψ was prepared at time t_1 . Conservation of probability in time requires that the operators $U(t_1, t_2)$ preserve the inner product, i.e., be *unitary*.

Of course, actual quantum theories encompasses more than what we have just described. However, it seems fair to say that realistic theories of quantum mechanics and quantum field theory contain at least the elements enumerated above.¹ Hence, we shall refer to these elements as defining the *standard formulation of quantum theory*.

To prepare the ground for the general boundary formulation let us think of the standard formulation as associating algebraic to geometric structures as follows. The geometric structures are points in time and intervals of time. The algebraic structures are states and transition amplitudes. To each point $t \in \mathbb{R}$ in time we associate a Hilbert space \mathcal{H}_t of states. These state spaces are simply copies of the usual state space \mathcal{H} and the labeling by a time is only a formality at this point. To each time interval $[t_1, t_2] \subset \mathbb{R}$ we associate a linear map $\rho_{[t_1, t_2]} : \mathcal{H}_{t_1} \otimes \mathcal{H}_{t_2} \rightarrow \mathbb{C}$,

¹ This characterization might not apply to certain frameworks for quantum field theory in curved spacetime, even for a fixed foliation. However, there is as yet no experimental test of quantum field theory in curved spacetime which could confirm such a framework.

called *amplitude map*.² This sends a pair of an initial and a final state (ψ, η) to the transition amplitude $\rho_{[t_1, t_2]}(\psi \otimes \eta) = \langle \eta | U(t_1, t_2) | \psi \rangle$. The amplitude map may be thought of as a map from the Hilbert space associated to the boundary $\partial[t_1, t_2] = t_1 \cup t_2$ of the time interval to the complex numbers. More generally, associate to a union of points in time $t_1 \cup \dots \cup t_n$ the product Hilbert space $\mathcal{H}_{t_1 \cup \dots \cup t_n} := \mathcal{H}_{t_1} \otimes \dots \otimes \mathcal{H}_{t_n}$. The composition rule may be seen as establishing a correspondence between geometric and algebraic operations: The geometric gluing of time intervals is put into correspondence with the algebraic composition of transition amplitudes. Concretely, the gluing $[t_1, t_3] = [t_1, t_2] \cup [t_2, t_3]$ is put into correspondence with the composition $\rho_{[t_1, t_3]}(\psi \otimes \eta) = \sum_i \rho_{[t_1, t_2]}(\psi \otimes \xi_i) \rho_{[t_2, t_3]}(\xi_i \otimes \eta)$, where $\{\xi_i\}$ denotes an ON-basis of \mathcal{H}_{t_2} .

The geometric-algebraic viewpoint becomes more compelling when we consider quantum field theory in (possibly curved) spacetime. Now the analogues of the points in time are spacelike hypersurfaces in spacetime. Again we have a state space \mathcal{H}_Σ associated with each spacelike hypersurface Σ . The analogues of the time-intervals are now spacetime regions bounded by two such hypersurfaces (an initial and a final one). Again we associate a linear amplitude map $\rho_M : \mathcal{H}_{\partial M} \rightarrow \mathbb{C}$ to such a region M with boundary $\partial M = \Sigma \cup \Sigma'$ and $\mathcal{H}_{\partial M} = \mathcal{H}_\Sigma \otimes \mathcal{H}_{\Sigma'}$. As before, this map sends a pair of initial and final state to the associated transition amplitude. And again, we have a composition rule associating to a gluing of spacetime regions the composition of the corresponding amplitude maps.

Let us go one step further: Associate state spaces to general hypersurfaces and amplitude maps to general spacetime regions. An immediate observation is that now different hypersurfaces might have not only different geometry, but even different topology. It is thus to be expected that the associated state spaces are not (naturally) isomorphic. Hence the previously formal distinction between them becomes a necessity. In this sense *the* state-space of a theory no longer exists. Another observation is that the boundary of a general spacetime region does not necessarily decompose into an “initial” and “final” hypersurface. Only in special cases it is possible to interpret the amplitude map $\rho_M : \mathcal{H}_{\partial M} \rightarrow \mathbb{C}$ for a region M with boundary ∂M as a transition amplitude between state spaces associated with boundary components. The composition rule can be generalized to this context as well as the notion of unitarity.

What we have described so far is the structural part of the *general boundary formulation of quantum theory*. We turn to its interpretational part later. See [1] for a more comprehensive account and [2] for a refined version of the system of rules or *axioms* involved.

2. Historical Remarks

2.1. Dirac’s attempt

Remarkably, the idea of associating amplitudes to general spacetime regions already appears in a paper by Dirac [3]. Dirac introduces what he calls “generalized transformation functions”, which are essentially the same as the generalized amplitudes considered here. What is more, he even proposes the spacetime gluing rule. However, his idea seems to have not been pursued at the time.³ This is not surprising, for several reasons:

- (i) The lack of need for such a formulation.
- (ii) The technical difficulties in realizing the proposal.
- (iii) The lack of a physical interpretation of the generalized amplitudes.

Let us elaborate on these reasons in turn. Concerning point (i), it turned out that non-relativistic quantum mechanics as well as quantum field theory get along very well with the

² The second tensor factor in the domain of $\rho_{[t_1, t_2]}$ should really be the dual space $\mathcal{H}_{t_2}^*$ of \mathcal{H}_{t_2} . This is because it represents a “bra”-vector in contrast to the first argument which represents a “ket”-vector. For simplicity of presentation, we gloss over this fact here as well as in the following.

³ Indeed, parts of this paper appear as well in Dirac’s monograph on quantum mechanics [4]. However, the part on “generalized transformation functions” is missing there.

usual type of transition amplitudes. Indeed, it is only in quantum gravity that one should expect this to no longer to be the case. In this sense Dirac's proposal was certainly ahead of its time. We will elaborate on this point later.

Concerning point (ii), standard quantization prescriptions rely on initial value problems. Since the differential equations of the classical theory are generally hyperbolic, this is normally ensured by considering the space of configuration data and its first derivatives on spacelike hypersurfaces. More general hypersurfaces do not admit a correspondence between classical solutions and boundary data of such a simple form. Furthermore, most quantization prescriptions describe time-evolution in an infinitesimal fashion. Exponentiation then leads to a spacelike hypersurface sweeping out a region of spacetime of interest, yielding the associated time-evolution operator. There is no analogous way to describe a general spacetime region and its associated amplitude. These two problems require a considerable modification of quantization prescriptions. This is probably the chief technical difficulty of the general boundary formulation.

Concerning point (iii), it is not clear how a general amplitude should give rise to a probability. Remarkably, Dirac himself, in the last paragraph of [3], attempted a probability interpretation, which unfortunately seems to be untenable. What is more, one might think that crucial consistency properties such as probability conservation require a temporal ordering of states, hence rendering any attempt at a consistent probability interpretation futile. While this is probably the most important a priori objection to the general boundary formulation it turns out to be unfounded. We will come to the probability in the next section.

2.2. Topological quantum field theory

A mathematical abstraction of the framework we have described so far is known as *topological quantum field theory*, see e.g. [5]. This arose in the 1980s and was strongly inspired by the path integral approach to quantum field theory. The latter goes back to Feynman's seminal paper [6] which in turn was inspired by Dirac's [3]. However, Feynman himself did not write anything about the generalized amplitudes.

Since topological quantum field theory is a mathematical framework the three reasons mentioned above for the lack of success of Dirac's idea do not apply to it. Concerning point (i), there are indeed interesting applications. Most notably, topological quantum field theory has given rise to a whole new branch of algebraic topology including the discovery of new invariants of knots and of 3-manifolds. While it is also applied to models in mathematical physics, these are toy models or auxiliary models where the technical difficulties referred to in point (ii) do not occur. These models also do not possess or require a direct interpretation in the sense of point (iii).

3. Probability Interpretation

We turn now to the interpretational part of the general boundary formulation. In the center stands the interpretation of generalized amplitudes as giving rise to physical probabilities. Probabilities in quantum theory are generally *conditional probabilities*. More specifically, such a probability usually depends on two type of data: Data that describes *knowledge* or *preparation* and data that describes a *question* or *observation*. In the simplest case we are looking for the probability to observe a specific state given that some other specific state was prepared.

In the general boundary formulation the dependence of probabilities on these two types of data is preserved. Consider a process taking place in a spacetime region M with boundary ∂M . Then, both type of data are encoded through closed subspaces of the state space $\mathcal{H}_{\partial M}$. Let $\mathcal{S} \subset \mathcal{H}_{\partial M}$ represent *preparation* or *knowledge*, and $\mathcal{A} \subset \mathcal{H}_{\partial M}$ represent *observation* or the *question*. The probability that the system is described by \mathcal{A} given that it is described by \mathcal{S} is:

$$P(\mathcal{A}|\mathcal{S}) = \frac{|\rho_M \circ P_{\mathcal{S}} \circ P_{\mathcal{A}}|^2}{|\rho_M \circ P_{\mathcal{S}}|^2}. \quad (1)$$

Here, P_S and P_A are the orthogonal projectors onto the respective subspaces and \circ represents composition of maps. Hence, the expressions in numerator and denominator that the norm square is taken of are linear maps $\mathcal{H}_{\partial M} \rightarrow \mathbb{C}$. The norm of such a map is defined here as follows.⁴ Let $\alpha : \mathcal{H}_{\partial M} \rightarrow \mathbb{C}$ be a bounded linear map. Then there exists $\xi \in \mathcal{H}_{\partial M}$ such that $\alpha(\psi) = \langle \xi, \psi \rangle \quad \forall \psi \in \mathcal{H}_{\partial M}$. Define $|\alpha| := |\xi|$.

$P(\mathcal{A}|\mathcal{S})$ has the properties expected of a (quantum mechanical) probability:

- By construction $P(\mathcal{A}|\mathcal{S})$ takes values in the interval $[0, 1]$.⁵
- Given two mutually exclusive observations encoded by orthogonal subspaces \mathcal{A}_1 and \mathcal{A}_2 the respective probabilities are additive, i.e., $P(\mathcal{A}_1 \oplus \mathcal{A}_2|\mathcal{S}) = P(\mathcal{A}_1|\mathcal{S}) + P(\mathcal{A}_2|\mathcal{S})$.
- The probability for an arbitrary outcome is $P(\mathcal{H}_{\partial M}|\mathcal{S}) = 1$ for any \mathcal{S} .
- If $\mathcal{A} \subseteq \mathcal{B} \subseteq \mathcal{C} \subset \mathcal{H}_{\partial M}$ (read: \mathcal{A} implies \mathcal{B} implies \mathcal{C}) we have the chain rule $P(\mathcal{A}|\mathcal{C}) = P(\mathcal{A}|\mathcal{B})P(\mathcal{B}|\mathcal{C})$.

To see how the expression (1) reduces to a standard transition probability, consider a region that is given by a time interval $[t, t']$. Thus, $\mathcal{H}_{[t, t']} = \mathcal{H}_t \otimes \mathcal{H}_{t'}$ and $\rho_M(\psi \otimes \eta) = \langle \eta | U(t' - t) | \psi \rangle$ as explained above. We want to calculate the probability that η is observed given that ψ was prepared. The preparation corresponds to the subspace $\mathcal{S} = \psi \otimes \mathcal{H}_{t'} \subset \mathcal{H}_{[t, t']}$ while the observation corresponds to the subspace $\mathcal{A} = \mathcal{H}_t \otimes \eta \subset \mathcal{H}_{[t, t']}$. It then turns out that formula (1) yields $P(\mathcal{A}|\mathcal{S}) = |\langle \eta | U(t' - t) | \psi \rangle|^2$ as required. For more complex examples of how (1) recovers the correct probabilities of standard quantum theory see [1].

Note a slight difference to the previous presentation of the probability interpretation in [1]. There, the subspace \mathcal{A} was restricted to be a subspace of \mathcal{S} as well. Lifting this restriction represents more a formal than a physical difference. Conceptually, making \mathcal{A} a subspace of \mathcal{S} just means taking into account the knowledge about the measurement when the question is asked. In particular, if P_S and P_A commute we can replace \mathcal{A} by $\mathcal{A} \cap \mathcal{S}$ without any change to $P(\mathcal{A}|\mathcal{S})$.

A property that is central to the consistency of the probability interpretation of quantum theory is *probability conservation*. Usually, this refers to conservation of probability *in time*. The present probability interpretation allows to extend this to a more general notion of probability conservation *in spacetime*. Consider a spacetime region M and an adjacent region N that we can think of as “deforming” M to $M' = M \cup N$.⁶ The amplitude map $\rho_N : \mathcal{H}_{\partial N} \rightarrow \mathbb{C}$ associated with N induces a map $\tilde{\rho} : \mathcal{H}_{\partial M} \rightarrow \mathcal{H}_{\partial M'}$. Now let $\mathcal{S} \subset \mathcal{H}_M$ and $\mathcal{A} \subset \mathcal{H}_M$ be subspaces determining a measurement in the sense discussed above. Define the subspaces $\mathcal{S}' := \tilde{\rho}(\mathcal{S}) \subset \mathcal{H}_{M'}$ and $\mathcal{A}' := \tilde{\rho}(\mathcal{A}) \subset \mathcal{H}_{M'}$. Then $P(\mathcal{A}|\mathcal{S}) = P(\mathcal{A}'|\mathcal{S}')$, i.e., the probability for observing \mathcal{A} given \mathcal{S} on ∂M is the same as that for observing \mathcal{A}' given \mathcal{S}' on $\partial M'$. Probability is conserved for “evolution” through the spacetime region N . For a more detailed discussion of this example, see [1]. If M is a time interval $[t_1, t_2]$ and N an adjacent time interval $[t_2, t_3]$ we recover the standard notion of probability conservation in time as a special case.

4. The general boundary formulation as an extension of quantum theory

The emphasis on spacetime might lead one to think of the general boundary formulation as a generalization of quantum field theory rather than quantum theory as such. However, quantum field theory can be reduced to the standard formulation of quantum theory while the general

⁴ There are a few subtleties that we are not detailing here. In particular, ρ_M is generically not bounded. Thus, \mathcal{S} must be “small enough” such that $\rho_M \circ P_S$ is bounded. This condition is satisfied in standard situations.

⁵ It might happen that the denominator is zero. In this case the numerator is also zero and $P(\mathcal{A}|\mathcal{S})$ is undefined. Physically this means that the knowledge encoded in \mathcal{S} does not correspond to any allowed process.

⁶ A technical definition of “deformation” could be: N should be contractible onto (a part of) the boundary of M .

boundary formulation cannot.⁷ This is why we prefer to see it as an extension of quantum theory itself. On the other hand, if we take spacetime to be the real line of time, we get back exactly the standard formulation of quantum theory (plus a more general probability interpretation). In this sense it is a special case of the general boundary formulation. Insofar quantum field theory is also trivially encompassed by the general boundary formulation. However, the conjecture is that realistic quantum field theories can be extended to quantum field theories based on the general boundary formulation with spacetime being taken to be what it is, rather than just a time axis. For examples and more details on the application to quantum field theory, see [7, 1, 8, 2].

It is clear already that the nature of the spacetime regions and hypersurfaces considered must depend heavily on the theory under consideration. As already discussed, in non-relativistic quantum mechanics they would be intervals and points on the real line (representing time). In standard quantum field theory they would be pieces of Minkowski spacetime. (Interestingly, one can try to use such a spacetime picture also in non-relativistic quantum mechanics, leading to effects otherwise typical only of quantum field theory [9].) In quantum field theory in curved spacetime they would be pieces of spacetime with a general Lorentzian metric.

General relativity teaches us that the metric is a dynamical field just like, say, the electromagnetic field. Hence, quantum gravity should be defined on spacetime regions and hypersurfaces without prescribed metric. This is sometimes referred to as *background independence*. Hence, spacetime regions and hypersurfaces should be merely differentiable manifolds. Indeed, a chief virtue of the general boundary formulation is that it admits such background independent theories.⁸

5. Towards quantum gravity

5.1. The quantum cosmology problem

A main motivation for the general boundary formulation comes from quantum gravity [10, 11]. We illustrate this with a well known problem that we shall call the *quantum cosmology problem*. If we look naively at standard quantum (field) theory as a description of our world, a state describes the whole universe at a given time (or spacelike hypersurface). Of course, we are usually interested in describing specific, localized systems and do not want to bother with all the rest of the universe. Quantum field theory allows us to do precisely that, telling us that distant systems can be treated as independent. Underlying this are powerful properties such as *causality* and *cluster decomposition*. In most cases we can accurately describe a local system as if it was living alone in an otherwise empty Minkowski universe.

In quantum gravity there is no metric background to separate systems. What is worse, diffeomorphism gauge symmetry makes any kind of (even relative) localization difficult. In particular, there is no causality or cluster decomposition property from the outset. Hence, at least a priori we cannot avoid that states are now really states of the whole universe. Apart from technical problems this also prompts deep conceptual problems such as to the meaning of quantum theory without an outside observer. It seems we have to do *quantum cosmology*.

While it might very well be that the mentioned problem can be solved within the standard formulation of quantum theory, it can be avoided in the general boundary formulation. State spaces, amplitudes and probabilities referring to *local* regions of spacetime allow to describe their physics independent of the physics outside. In particular, there is now no difficulty in placing the observer outside of the quantum mechanical process under consideration. Indeed,

⁷ But recall footnote 1.

⁸ Sometimes “background independence” is taken to mean also that there is no differentiable structure or not even the structure of a (topological) manifold. The latter case would not fit into the general boundary formulation, at least not in its present form.

this suggests that we should *only* allow local regions in a quantum theory of gravity. Infinitely extended regions or regions “wrapping around the universe” would not be admissible.

5.2. Graviton scattering: A scenario

To understand more concretely how predictions in a quantum theory of gravity could be formulated we consider the following semiclassical scenario. Consider a 4-ball shaped region $M = B^4$ in spacetime with boundary $\partial M = S^3$. We suppose that there is a semiclassical sector of the theory such that M may be described as a piece of Minkowski spacetime with small fluctuations. Formalizing this, the state space associated with the boundary of M contains a sector \mathcal{H}_{lin} describing this regime and can be decomposed as $\mathcal{H}_{\partial M} = \mathcal{H}_{\text{lin}} \oplus \mathcal{H}_{\text{nlin}}$.

It should now be expected that \mathcal{H}_{lin} is (approximately) a Fock space with graviton states. What is more, learning from a related quantum field theory example [8] we expect it to (approximately) factorize into in- and out-states, $\mathcal{H}_{\text{lin}} = \mathcal{H}_{\text{in}} \otimes \mathcal{H}_{\text{out}}$. Now pick an n -graviton state $\psi_{p_1, \dots, p_n; \text{in}}$ in \mathcal{H}_{in} and an m -graviton state $\psi_{q_1, \dots, q_m; \text{out}}$ in \mathcal{H}_{out} . The associated scattering probability (density) would be given by $P(\mathcal{A}|\mathcal{S})$ with $\mathcal{A} = \psi_{p_1, \dots, p_n; \text{in}} \otimes \mathcal{H}_{\text{out}}$ and $\mathcal{S} = \mathcal{H}_{\text{in}} \otimes \psi_{q_1, \dots, q_m; \text{out}}$. A few remarks are in order:

- Although the scenario discussed is that of a *semiclassical* description, there is no approximation or reduction performed before quantization. All objects under consideration would be objects of the full quantum theory.
- The factorization of the subspace \mathcal{H}_{lin} into in- and out-states should not be expected to extend to a factorization of the full state space $\mathcal{H}_{\partial M}$.
- The detailed results will depend on how exactly we choose \mathcal{H}_{lin} in $\mathcal{H}_{\partial M}$, in which way it approximates a Fock space, up to which energies, etc. One might conjecture that these ambiguities are related to the renormalization ambiguities of perturbative quantum gravity.

For first steps in applying (so far only the structural part of) the general boundary formulation in a loop quantum gravity / spin foam context see [11, 12, 13, 14].

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- [1] R. Oeckl, *General boundary quantum field theory: Foundations and probability interpretation*, Preprint hep-th/0509122, 2005.
- [2] R. Oeckl, *Two-dimensional quantum Yang-Mills theory with corners*, Preprint hep-th/0608218, 2006.
- [3] P. A. M. Dirac, *The Lagrangian in Quantum Mechanics*, Phys. Z. Sowjetunion **3** (1933), 64–72.
- [4] P. A. M. Dirac, *The Principles of Quantum Mechanics*, 4 ed., Oxford University Press, Oxford, 1958.
- [5] M. Atiyah, *Topological quantum field theories*, Inst. Hautes Études Sci. Publ. Math. (1989), no. 68, 175–186.
- [6] R. P. Feynman, *Space-time approach to non-relativistic quantum mechanics*, Rev. Mod. Phys. **20** (1948), 367–387.
- [7] R. Oeckl, *States on timelike hypersurfaces in quantum field theory*, Phys. Lett. **B 622** (2005), 172–177, hep-th/0505267.
- [8] R. Oeckl, *General boundary quantum field theory: Timelike hypersurfaces in Klein-Gordon theory*, Phys. Rev. **D 73** (2006), 065017, hep-th/0509123.
- [9] R. Oeckl, *A “general boundary” formulation for quantum mechanics and quantum gravity*, Phys. Lett. **B 575** (2003), 318–324, hep-th/0306025.
- [10] R. Oeckl, *Schrödinger’s cat and the clock: Lessons for quantum gravity*, Class. Quantum Grav. **20** (2003), 5371–5380, gr-qc/0306007.
- [11] F. Conrady, L. Doplicher, R. Oeckl, C. Rovelli, and M. Testa, *Minkowski vacuum in background independent quantum gravity*, Phys. Rev. **D 69** (2004), 064019, gr-qc/0307118.
- [12] R. Oeckl, *The general boundary approach to quantum gravity*, Proceedings of the First International Conference on Physics (Tehran, 2004), Amirkabir University, Tehran, 2004, pp. 257–265, gr-qc/0312081.
- [13] C. Rovelli, *Quantum gravity*, Cambridge University Press, Cambridge, 2004.
- [14] C. Rovelli, *Graviton propagator from background-independent quantum gravity*, Phys. Rev. Lett. **97** (2006), 151301, gr-qc/0508124.